APPENDIX 1

Program for Baselining, Normalizing, Interpolating Then

Calculating Spectral Overlap Integrals

```
C       This program has a non-standard DO WHILE loop

        INTEGER NPTS, NMAX, ROWS, ITER
        INTEGER EOF1, FLERR1, FLERR2
        INTEGER EOF2, FLERR3, FLERR4
        INTEGER EOF3, FLERR5, FLERR6
        INTEGER FLERR7
        INTEGER i,j
        CHARACTER*30 fname1, fname2, fname3, fname4
        CHARACTER*30 fname5, fname6, fname7
        PARAMETER(NMAX=3500, LAMDA=601)
        REAL x,xx1 (NMAX) ,yy1 (NMAX),INTERV1
        REAL xx2 (NMAX) ,yy2 (NMAX), INTERV2

        REAL xx3 (NMAX), yy3 (NMAX),INTERV3
        REAL yi1 (NMAX), yi2 (NMAX), yi3 (NMAX), yc (NMAX)
        REAL area
        CHARACTER*1 SUBSTR, INITAR, LIGHT, INTMED

        FLERR1=0
        FLERR2=0
        FLERR3=0
        FLERR4=0
        FLERR5=0
        FLERR6=0
        FLERR7=0
        EOF1=0
        EOF2=0
        EOF3=0
        INTERV1=0
        INTERV2=0
        INTERV3=0
        area=0

        write(*,*) 'Do you wish to output intermediate files? (Y/N)'
        read(*,'(A)') INTMED

        write(*,*) 'Do you wish to process a substrate file? (Y/N)'
        read(*,'(A)') SUBSTR

        IF ((SUBSTR.EQ.'Y') .OR. (SUBSTR.EQ.'y')) THEN
```

```fortran
      ITER=0
      do 5 ITER=1, NMAX
            xx1 (ITER)=0
            yy1 (ITER)=0
            yi1 (ITER)=0
5         continue

      write(*,*) 'Enter the name of the input substrate file:'
      read(*,' (A)') fnamel

      open
      (UNIT=11,FILE=fnamel,STATUS='OLD',IOSTAT=FLERR1,E
      RR=101)

      ROWS=0

      do while  ((EOF1.EQ.0) .AND. (ROWS.LT.NMAX))
            ROWS=ROWS+1
            Read (11,*,IOSTAT=EOF1) xx1 (ROWS), yy1 (ROWS)
      end do

      close (UNIT=11)
      NPTS=0

      IF (EOF1.NE.0) THEN
            NPTS=ROWS-1
            write(*,'(I4,1X,A12)') NPTS, 'points read.'
      ELSE
            NPTS=ROWS
            write(*,'(A28, I4, A12)') 'Too many data points! First',
      +                              NMAX,' points read...'
      END IF

      call baseln(yy1,NPTS)

      IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

            write(*,*) 'Enter the name of the output substrate file:'
            read(*,' (A)') fname2
            open
      (UNIT=12,FILE=fname2,STATUS='NEW',IOSTAT=FLERR2,
      ERR=102)

            write(*,*) 'Writing data...'

      END IF
```

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```
        x=0
        i=0
        j=0

        do 12 i=1, LAMDA

                x= (i-1)+200

                call locate(xx1,NPTS,x,j)

                if ((j.eq.0). OR. (j.eq.NPTS)) then
                        INTERV1=0
        else
                INTERV1= ((yyl(j+1)-yyl(j)) / (xx1(j+1) – xx1(j))) *
        (x-xxl(j))
        +                +yyl(j)

        end if

        yi1 (i)=INTERV1

        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

                if ((j.eq.0) .OR. (j.eq.NPTS)) then
                GO TO 12
                else
                write(12,'(1x, f7.2,i6,3f12.2)')x,j,xxl(j),xxl(j+1),
        +                INTERV1

                        endif

        END IF

12              continue
        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
                close (UNIT=12)

        END IF

        ELSE
                ITER=0
                do 14 ITER=1, LAMDA
                        yi1 (ITER) =1
14                              continue

        ENDIF
```

```
      write(*,*) 'Do you wish to process an initiator file? (Y/N)'
      read(*,'(A)') INITAR

5     IF ((INITAR.EQ.'Y') .OR. (INITAR.EQ.'y')) THEN

          ITER=0

      do 15 ITER=1,NMAX
10        xx2 (ITER) =0
          yy2 (ITER) =0
          yi2 (ITER) =0
15            continue

15    write(*,*) 'Enter the name of the initiator file:'
      read(*,'(A)') fname3

      open
      (UNIT=13,FILE=fname3,STATUS='OLD',IOSTAT=FLERR3,
20    ERR=103)

      ROWS=0

      do while ((EOF2.EQ.0) .AND. (ROWS.LT.NMAX))
25        ROWS=ROWS+1
          read(13,*,IOSTAT=EOF2) xx2 (ROWS), yy2 (ROWS)
      end do

      close (UNIT=13)
30
      NPTS=0

      IF (EOF2.NE.0) THEN
          NPTS=ROWS-1
35        write(*,1(14,1X,A12)') NPTS,'points read.'
      ELSE
          NPTS=ROWS
          write (*,'(A28,I4,A12)') 'Too many data points! First ',
      +                       NMAX,' points read...'
40        END IF
          call baseln (yy2,NPTS)

      IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

45        write(*,*) 'Enter the name of the output initiator file: '
          read(*,'(A)') fname4
```

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```
                open
        (UNIT=14,FILE=fname4,STATUS='NEW',IOSTAT=FLERR4,
        ERR=104)

                write(*,*) 'Writing data...'

        END IF
        x=0
        i=0
        j=0

        do 22 i=1,LAMDA
                x= (i-1)+200

                call locate (xx2,NPTS,x,j)
        if ((j.eq.0).OR. (j.eq.NPTS)) then
                        INTERV2=0
                else
                        INTERV2= ((yy2(j+1)-yy2(j)) / (xx2(j+1) – xx2
        (j))) * (x-xx2 (j))
        +                       +yy2 (j)
                end if
                yi2 (i)=INTERV2
                IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

                        if ((j.eq.0) .OR. (j.eq.NPTS)) then
                                GO TO 22
                        else
                                write(14,'(1x,f7.2,i6,3f12.2)') x, j, xx2
        (j),xx2 (j+1),
        +                               INTERV2

                        endif

                END IF

        22              continue

        IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

                close (UNIT=14)

        END IF
        ELSE

                ITER=0
```

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```fortran
      do 24 ITER=1,LAMDA
            yi2 (ITER)=1
24                continue

      ENDIF
      write(*,*) 'Do you wish to process a light source file? (Y/N)'
      read(*,'(A)') LIGHT

      IF ((LIGHT.EQ.'Y').OR. (LIGHT.EQ.'y')) THEN
            ITER=0
            do 25 ITER=1,NMAX
                  xx3 (ITER) =0
                  yy3 (ITER) =0
                  yi3 (ITER)=0
25                continue

      write(*,*) 'Enter the name of the light source file:'
      read(*,' (A)') fname5

      open
      (UNIT=15,FILE=fname5,STATUS='OLD',IOSTAT=FLERR5,
      ERR=105)

      ROWS=0

      do while ((EOF3.EQ.0) .AND. (ROWS.LT.NMAX))
            ROWS=ROWS+1
            read(15,*,IOSTAT=EOF3) xx3 (ROWS), yy3 (ROWS)
      end do

      close (UNIT=15)

      NPTS=0
      IF (EOF3.NE.0) THEN
            NPTS=ROWS-1
            write(*,1 (14,1X,A12)1) NPTS, 'points read.'
      ELSE
            NPTS=ROWS
            write (*,' (A28,I4,A12)') 'Too many data points! First ',
+                              NMAX,' points read...'
      END IF

      call norm (yy3,NPTS)

      IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

            write(*,*) 'Enter the name of the light source output file:'
```

```
                read(*,' (A)') fname6
                open
        (UNIT=16,FILE=fname6,STATUS='NEW',IOSTAT=FLERR6,
        ERR=106)

                write(*,*) 'Writing data...'

        END IF
        x=0
        i=0
        j=0

        do 32 i=1,LAMDA
                x= (i-1)+200
                call locate (xx3,NPTS,x,j)
                if ((j.eq.0) .OR. (j.eq.NPTS)) then
                        INTERV3=0
                else
                        INTERV3= ((yy3(j+1) – yy3(j)) / (xx3(j+1) –
        xx3(j))) * (x-xx3 (j))
        +                                               +yy3 (j)
                end if
                yi3 (i) =INTERV3
                IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

                        if ((j.eq.0).OR. (j.eq.NPTS)) then
                                GO TO 32
                        else
                        write(16,'(1x,f7.2,i6,3f12.2)') x,j,xx3 (j),xx3 (j+1),
        +                                               INTERV3
                        endif

        END IF

        32          continue
        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

                close (UNIT=16)

        END IF

        ELSE
        ITER=0

        do 34 ITER=1,LAMDA
                yi3 (ITER) –1
        34                          continue
```

```
            ENDIF

            ITER=0

            DO 40 ITER=1,LAMDA
                  yc (ITER)=0
            40          CONTINUE

            DO 55 i=1,LAMDA
                  yc (i) −yi1 (i)*yi2 (i)*yi3 (i)
            55          CONTINUE

            write(*,*) 'Enter the filename for cumulative data:'
            read (*,'(A)') fname7
            open
            (UNIT=17,FILE=fname7,STATUS='NEW',IOSTAT=FLERR7,
            ERR=107)
            write(*,*) 'Writing data...'

            CALL integ (yc,LAMDA,area)

            write(*,'(1X,A26,All,F12.6)') 'The area under the product',
            +'curve is:',area

            write(17,'(1X,A26,A11,F12.6)') 'The area under the product',
            +' curve is: ',area

            DO 60 i=1,LAMDA
                  x= (i-1)+200
                  write(17,' (1X,F6.1,2F11.2,F11.4,E15.6)') x,yi1 (i),yi2
            (i),
            +                        yi3 (i) ,yc (i)
            60          CONTINUE

            close (UNIT=17)

            101    IF (FLERR1 .NE. 0) THEN
                  write(*,*) 'Unable to open substrate file!'
            END IF

            102    IF (FLERR2 .NE. 0) THEN
                  write(*,*) 'Unable to create substrate output file!'
            END IF

            103    IF (FLERR3 .NE. 0) THEN
                  write(*,*) 'Unable to open initiator file!'
```

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END IF

```
104     IF (FLERR4 .NE. 0) THEN
        write(*,*) 'Unable to create initiator output file!'
END IF

105     IF (FLERR6 .NE. 0) THEN
        write(*,*) 'Unable to open light source file!'
END IF

106     IF (FLERR6 .NE. 0) THEN
        write(*,*) 'Unable to create light source output file!'
END IF

107     IF (FLERR7 .NE. 0) THEN
        write(*,*) 'Unable to create cumulative output file!'
END IF

write(*,*) 'Program exiting normally...'

END

SUBROUTINE locate (xx,n,x,j)
INTEGER j,n
REAL x,xx (n)
INTEGER j1,jm,ju
J1=0
ju=n+1
10              if (ju-j1.gt.1) then
        jm= (ju+j1) /2
        if ((xx (n).ge.xx (1)) .eqv. (x.ge.xx (jm))) then
                j1=j m
        else
                ju=jm
        endif
goto 10
endif
if (x.eq.xx (1))then
        j=1
else if (x.eq.xx(n))then
        j=n-1
else
        j=j1
endif
return END

SUBROUTINE baseln (yy,N)
```

```
            INTEGER N, i
            REAL yy (N), minno, temp

  5         minno=yy (1)
            i=0
            temp=0

            DO 10 i=2,N
 10              IF (yy (i) .LT. minno) THEN
                     minno=yy (i)
                 END IF
            10          CONTINUE

 15         i=0

            DO 20 i=1,N
                 temp=yy (i)-minno
                 yy (i)=temp
 20         20          CONTINUE

            END

            SUBROUTINE norm (yy,N)

 25         INTEGER N, i
            REAL yy (N),maxno,temp

            maxno=yy (1)
 30         i=0
            temp=0

            DO 5 i=2,N
                 IF (yy(i).GT.maxno) THEN
 35                  maxno=yy (i)
                 END IF
            5           CONTINUE

            i=0
 40
            DO 10, i=1,N
                 temp=yy (i)/maxno
                 yy (i)=temp
            10          CONTINUE
 45
            END
```

```fortran
        SUBROUTINE integ (yy,N,area)

        INTEGER N,i
        REAL yy (N),sum,area
5
        i=0
        sum=0
        area=0

10      DO 10 i=1,N-1
              sum=sum+ (yy(i)+yy (i+1))*0.5
        10          CONTINUE

        area=sum/100000
15
        END
```

Program to create uniformly spaced csv data from unevenly spaced
tabular data

5

```c
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#define NMAX 3501
#define STRMAX 151
#define FNMAX 81
#define OUTPTS 801

void locate(float xx[], unsigned long n, float x, unsigned long *j);
void norm(float xx[], unsigned long int n);
void baseline(float xx[], unsigned long int n);

int main()
{
char fnamein(FNMAX], string[STRMAX], *str, ptr,
fnameout[FNMAX], another;
float xdata(NMAX], ydata[NMAX], xinter[OUTPTS+1],
yinter[OUTPTS+1];
unsigned long int index, i, j;
int choice;
FILE *fpin, *fpout;

another = 'Y';

do {
    for (i = 0; i <= NMAX-1; i++) {
        xdata [i] = 0;
            ydata [i] = 0;
};

    for (i = 0; i <= OUTPTS; i++) {
        xinter [i] = 0;
            yinter (i] = 0;
};

printf("Enter name of the input file (80 chars max, no spaces): ");
scanf("%s", fnamein);

printf("File name is %s\n",fnamein);

fpin = fopen(fnamein,"r");

if (fpin == NULL) {
```

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```c
            printf("Cannot open %s\n",fnamein);
            exit(1);
        };

    index = 1;

    while (1) {
        str_ptr = fgets(string,STRMAX-1,fpin);
        if(str_ptr == NULL)
            break;
        if (index == NMAX)
            break;
        sscanf (string, "%f %f" , &xdata [index] , &ydata [index]);
        index++;
    };

    f close (fpin);

    if((index == NMAX) && (str_ptr != NULL)) {
        index--;
        printf("Too many data points! Using first %d points
only...\n",index);
    }
    else {
        index--;
        printf("%d points read...\n",index);
    };

    printf("\nEnter option for data processing\n");
    printf("1: Normalize the data after interpolation\n");
    printf("2: Baseline the data after interpolation\n");
    printf("3: First interpolate, then baseline and finally ");
    printf("normalize the data\n");
    printf("4: Simply interpolate the data\n");
    printf("5: Simply normalize the data\n");
    printf("6: Simply baseline the data\n");
    printf("or\n");
    printf("0: to exit the program without any data processing\n");
    printf("\nEnter option (0-6): ");
    scanf("%d",&choice);

    if (choice == 0)
        exit(2);

    printf("\nEnter name of the output file (80 chars max, no spaces): ");
    scanf("%s",fnameout);

    printf("File name is %s\n",fnameout);
```

```
fpout = fopen(fnameout,"w");

if (fpout == NULL) {
    printf("Cannot open %s\n",fnameout);
    exit(3);
};

for(i = 1; i <= OUTPTS; i++) {
    xinter[i] = 200+((float)i-1);
    locate(xdata,index,xinter[i],&j);
    if ((j == 0) || (j == index))
        yinter[i] = 0;
    else
        yinter [i] = (xinter [i] -xdata [j ]) * ((ydata (j+1] -ydata [j ]) /
                (xdata [j+1] -xdata [j ])) +ydata [j ] ;
};

if ((choice == 2) || (choice == 3)) {
    baseline(yinter,OUTPTS);
};

if (choice == 6) {
    baseline(ydata,index);
};

if ((choice == 1) || (choice == 3)) {
    norm(yinter,OUTPTS);
};

if (choice == 5) {
    norm(ydata,index);
};

if ((choice >= 1) && (choice <= 4)) {
    for (i = 1; i <= OUTPTS-1; i++) {
        fprintf(fpout,"%13.5E, ",yinter[i]);
    };
    fprintf(fpout,"%13.5E\n",yinter[OUTPTS]);
    }
    else
        if ((choice == 5) || (choice == 6)) {
                for (i = 1; i <= index-1; i++)
                fprintf(fpout,"%13.5E, ",ydata[i]);
                };
                fprintf(fpout,"%13.5E\n",ydata[index]);
        };

    fclose(fpout);
```

37

```c
            printf("File %s written.\n\n",fnameout);
            printf("Process another file (Y/y/N/n)?: ");
            scanf("%ls",&another);
        }    while (another == 'Y' || another == 'y');

        printf("Exiting...\n");
        return(0);
        }                        .

        void locate(float xx[], unsigned long n, float x, unsigned long *j)
        {
        unsigned long ju,jm,jl;
        int ascnd;

        jl=0;
        ju=n+1;
        ascnd=(xx[n] >= xx[1]);
        while (ju-jl > 1) {
            jm=(ju+j l) >> 1;
            if (x >= xx [j m] == ascnd)
                jl=jm;
            else
                ju=jm;
        }
        if (x == xx [1] )
            *j=1;
        else if (x == xx[n])
            *j=n-1;
        else
            *j=jl;
        }

        void norm(float xx[], unsigned long int n)
        {
        unsigned long int i;
        float maxdata, temp;

        maxdata = xx [1] ;
        temp = 0;

        for(i = 2; i <= n; i++) {
            if(xx[i] > maxdata)
                maxdata = xx[i];
        };

        for(i = 1; i <= n; i++) {
            temp = xx[i]/maxdata;
            xx [i] = temp;
        };
```

```
}

void baseline(float xx[], unsigned long int n)
{
unsigned long int i;
float mindata, temp;
mindata = xx [ 1 ] ;
temp = 0;

for(i = 2; i <= n; i++) {
    if(xx[i] < mindata)
        mindata = xx [i] ;
};

for(i = 1; i <= n; i++) {
    temp = xx(i] - mindata;
    xx(i] = temp;
};
}
```

APPENDIX 3

Program for Determining Strength of Wavelength Response in a Region

```c
#include
<stdio.h>
#include
<stdlib.h>
#include
<math.h>

#define NMAX
3501
#define STRMAX
151
#define FNMAX
81
#define OUTPTS
801

void locate(float xx[], unsigned long n, float x,
unsigned long *j);
void norm(float xx[], unsigned long
int n);
void baseline(float xx[], unsigned
long int n);
void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
  float *area);

int
main()
{
  char fnamein[FNMAX], string[STRMAX], *str_ptr,
fnameout[FNMAX], another;
  float xdata[NMAX], ydata[NMAX], xinter[OUTPTS+1],
yinter[OUTPTS+1];
  float
totalarea,aA,aB,aC,aD,aE,aF,aG,aH,aI,aJ,a
K;
  unsigned long int index, i,
j;
  int choice;
  FILE *fpin,
*fpout;
```

```
another = 'Y';

    printf("Contact Rajdeep S. Kalgutkar, SRC-CRC 7-3003, for
further info\n");

  do {
    for (i = 0; i <= NMAX-1;
i++) {
      xdata[i]=0;
      ydata[i]=0;
    };

    for (i = 0; i <= OUTPTS;
i++) {
      xinter[i]=0;
      yinter[i]=0;
    };

    printf("\nEnter name of the input file (80 chars max, no
spaces): ");
    scanf("%s",fnamein);

    printf("File name is
%s\n",fnamein);

    fpin =
fopen(fnamein,"r");

    if (fpin ==
NULL) {
      printf("Cannot open %s.
Exiting...\n",fnamein);

exit(1);
    };

    index = 1;

    while (1) {
    str_ptr = fgets(string,STRMAX-
1,fpin);
      if(str_ptr == NULL)
        break;
      if(index == NMAX)
        break;
      sscanf(string,"%f
%f",&xdata[index],&ydata[index]);
```

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```c
    index++;
  };

  fclose(fpin);

  if((index == NMAX) && (str_ptr != NULL)) {
    index--;
    printf("Too many data points! Using first %d points
only...\n",index);
  }
  else {
    index--;
    printf("%d points
read...\n",index);
  };

  printf("\nEnter option for data
processing\n");
  printf("1: Simply interpolate the
data\n");
  printf("2: Normalize the data after
interpolation\n");
  printf("3: Baseline the data after
interpolation\n");
  printf("4: First interpolate, then baseline and finally
");
  printf("normalize the
data\n");
  printf("or\n");
  printf("0: to exit the program without any data
processing\n");
  printf("\nEnter option (0-
4): ");
  scanf("%d",&choice);

  if (choice == 0)

exit(2);

  printf("\nEnter name of the output file (80 chars max, no
spaces): ");
  scanf("%s",fnameout);

  printf("File name is
%s\n",fnameout);

  fpout =
```

```c
fopen(fnameout,"w");

    if (fpout ==
NULL){
        printf("Cannot open %s.
Exiting...\n",fnameout);

exit(3);
    };

    for(i = 1; i <= OUTPTS;
i++) {
        xinter[i] = 200+((float)i-
1);
        locate(xdata,index,xinter[i],&j);
        if((j == 0) || (j ==
index))
            yinter[i] = 0;
        else
            yinter[i]=(xinter[i]-xdata[j])*((ydata[j+1]-
ydata[j])/
            (xdata[j+1]-xdata[j]))+ydata[j];
    };

    if ((choice == 3) || (choice == 4)) {

baseline(yinter,OUTPTS);
    };

    if ((choice == 2) || (choice == 4)) {
        norm(yinter,OUTPTS);
    };


partinteg(yinter,51,OUTPTS,&totala
rea);


partinteg(yinter,51,101,&a
A);

partinteg(yinter,101,151,&
aB);

partinteg(yinter,151,201,&
aC);
```

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```c
partinteg(yinter,201,251,&
aD);

partinteg(yinter,251,301,&
aE);

partinteg(yinter,301,351,&
aF);

partinteg(yinter,351,401,&
aG);

partinteg(yinter,401,451,&
aH);

partinteg(yinter,451,501,&
aI);

partinteg(yinter,501,551,&
aJ);

partinteg(yinter,551,OUTPTS,&aK);

    fprintf(fpout,"The total area is:
%14.6E\n",totalarea);
    fprintf(fpout,"The area under region A is:
%6.2f%%\n",aA*100/totalarea);
    fprintf(fpout,"The area under region B is:
%6.2f%%\n",aB*100/totalarea);
    fprintf(fpout,"The area under region C is:
%6.2f%%\n",aC*100/totalarea);
    fprintf(fpout,"The area under region D is:
%6.2f%%\n",aD*100/totalarea);
    fprintf(fpout,"The area under region E is:
%6.2f%%\n",aE*100/totalarea);
    fprintf(fpout,"The area under region F is:
%6.2f%%\n",aF*100/totalarea);
    fprintf(fpout,"The area under region G is:
%6.2f%%\n",aG*100/totalarea);
    fprintf(fpout,"The area under region H is:
%6.2f%%\n",aH*100/totalarea);
    fprintf(fpout,"The area under region I is:
%6.2f%%\n",aI*100/totalarea);
    fprintf(fpout,"The area under region J is:
%6.2f%%\n",aJ*100/totalarea);
    fprintf(fpout,"The area under region K is:
%6.2f%%\n\n",aK*100/totalarea);
```

```c
    for (i = 1; i <= OUTPTS-1; i++) {
      fprintf(fpout,"%13.5E, ",yinter[i]);
    };
    fprintf(fpout,"%13.5E\n",yinter[i]);

    fclose(fpout);

    printf("File %s
written.\n\n",fnameout);
    printf("Process another file
(Y/y/N/n)?: ");
    scanf("%1s",&another);
  } while (another == 'Y' || another
== 'y');


printf("Exiting...\n
");

return(0
);
}

void locate(float xx[], unsigned long n, float x,
unsigned long *j)
{
  unsigned long ju,jm,jl;
  int ascnd;

  jl=0;

ju=n+1;
  ascnd=(xx[n] >= xx[1]);
  while (ju-jl > 1) {
    jm=(ju+jl) >> 1;
    if (x >= xx[jm] == ascnd)

jl=jm;
    else

ju=jm;
  }
  if (x == xx[1])
    *j=1;
  else if(x ==
```

```c
    xx[n])
      *j=n-
    1;
      else
        *j=jl;
    }

    void norm(float xx[], unsigned long
    int n)
    {
      unsigned long
    int i;
      float maxdata,
    temp;

     maxdata =
    xx[1];
      temp =
    0;

      for(i = 2; i <= n; i++) {
        if(xx[i] >
    maxdata)
          maxdata =
    xx[i];
      };

      for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
      };
    }

    void baseline(float xx[], unsigned
    long int n)
    {
      unsigned long
    int i;
      float mindata,
    temp;

      mindata = xx[1];
      temp =
    0;

      for(i = 2; i <= n; i++) {
        if(xx[i] <
```

```
mindata)
    mindata =
xx[i];
  };

  for(i = 1; i <= n; i++) {
    temp = xx[i] - mindata;
    xx[i] = temp;
  };
}

void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
  float *area)
{
  unsigned long
int i;
  float temp;

  temp =
0;

  for(i = x1; i <= x2 - 1; i++)
{
    temp = temp + (xx[i] + xx[i+1])/2;
  };

  *area = temp;
}
```

APPENDIX 4

SRC Curing Resource dB 4 Query Select2

```
5       Sub Initialize
                Dim ses ses As New NotesSession
                Dim db_db As NotesDatabase
                Dim view view As NotesView
                Dim note _notel As NotesDocument, note_note2 As NotesDocument
10              Dim i cnt As Integer, i add As Integer


        Set db db =ses ses.CurrentDatabase
        Set note notel=ses ses.DocumentContext


15      Redim Preserve arr WavelengthRegion(0) air WavelengthRegion(0) _ ""


                If note_notel.Selectionl(0) <> "" Or rwte_notel.Selection2(O) <> "" Then
                If note notel.Selectionl(0) <> "" Then
        Set view_view = db_db.GetView("By NoteID")

20
        If note notel.Selection2(0) <> ""Then
        Set note_note2=view_view.GetDocumentByKey(Right("00000000" &
        note_notel.Selection2(01, 8))
        Else
25      Set note note2 = view_view.GetDocumentByKey(Right("00000000" &
        note_notel.Selectionl(0), $))
        End If


        If Not (note_note2ls Nothing) Then
        If note note2.Hasltem('WavelengthRegion") Then
30      i_cnt = -1
        Forall vals In note_note2.WavelengthRegion
                If vals <> "" Then
                        i_cnt = i_cnt + 1
35                      Redim Preserve arr WavelengthRegion(i_cnt)
                        arr_WavelengthRegion(i cnt) = vals
                End If
        End Forall


40      End If
        End If End If


        If note notel.Type(0) = "S" Then
                Set view-View = db db.GetView("Substrate")
45      Elseif note _notel.Type(O) = "P" Then
        Set view-view = db_db.GetView("InitiatorSensitizer") Else
        Set view-view = db_db.GetView("LightSource") End If
```

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```
                    ' Set note note2 =view-view. GetFirstDocument

                    i_cnt = -1
        5           Do While Not (note note2 Is Nothing)
                    If note_note2.Name(0) <> "" Then
                    L add = True
                    If arr WavelengthRegion(0) <> "" Then
                    Ladd = False
        10          Forall valsl In note _note2.WavelengthRegion
                            Forall vals2 In arr_WavelengthRegion
                                If valsl = vals2 Then
                                    i_add = True
                                    Exit Forall
        15                      End If
                            End Forall

                            If Ladd Then
                                    Exit Forall
        20                  End If
                    End Forall
                    End If

                    If L add Then
        25                  i cnt = i cnt + 1
                            Redim Preserve arr_names(i cnt)
                            arr names(i_cnt) = note_note2.Name(O)
                        End If
                    End It
        30
                            Set note note2 = view-view. GetNextDocument(note_note2)
                    Loop

                    note        _notel .Names = arr_names
        35          End Sub

                    SRC Curing Resource dB 4 Query Select2 Save Agent

                    Sub Initialize
        40              Dim ses sesAs New NotesSession
                        Dim db_db As NotesDatabase
                        Dim view view As NotesView
                        Dim note_notel As NotesDocument, note_note2As NotesDocument

        45          Set db_db = ses ses.CurrentDatabase
                    Set note note) = ses ses.DocumentContext
```

```
Select Case note_notel.Type(0)
Case "S"
Set view view = db_db.GetView("(Substrate)")

Set note_note2=view view.GetDocumentByKey(note_notel.Substrate(0))

Case "P"
Set view-view db-db.GetView("(InitiatorSensitizer)")

Set note note2 -view view.GetDocumentByKey(note notel.PhotoInitiator(O))

Case "L"
Set view-view =db db.GetView("(LightSource)")

Set note_note2 = view_view.GetDocumentByKey(note_notel.LightSource(0))

End Select

If note_notel.MexWction(0) = "Add" Then
If note_notel.Selectionl (0) <> "" Then
Print "[!" + note notel.dbname(O) + "/QuerySelectionl?OpenForm&" &
note_notel.Selectionl (0) & "&" & note_note2.Noteld & ")"
Else
Print "[!" + note notel.dbname(0) + "/QuerySelectionl?OpenForm&" &
note_note2.Noteld & "]"
End If Elseif note notel.NextAction(O) = "Separate" Then
If note_notel.Selectionl(0) <> "" Then
Print "[/" + note notel.dbname(O) + "/QuerySelectionl?OpenForm&" &
note_notel.Selectionl(O) & "&" & note note2.Noteld & ")"
Else
Print "[!" + note notel.dbname(O) + "/QuerySelectionl?OpenForm&" &
note_note2.Noteld & ")"
End If
Elseif note _notel.NextAction(O) = "Separate" Then
If note _notel.Selection2(0) <> "" Then
Print "[/" + note notel.dbname(O) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection) (0) & "&" & note note).Selection2(0) & _
"&" & note_note2.Noteld & "]"
Elseif note notel.Selectionl(0) <> "" Then
Print- "[" + note notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selectionl (0) & "&" & note note2.Noteld & ")"
Else
Print "[/" + note_notel.dbname(O) + "lQuerySelectionResults?OpenForm&" &
note_noteMoteld & "]"
End If
Else
If note notel.Selection2(0) <> "" Then
```

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```
       Print "[/" + note_notel.dbname(0) + "/QuerySelectionOverlayResults?OpenForm&" &
       note_notel.Selectionl(0) & "&" & note_notel.Selection2(0) &
       "&" & note_note2.Noteld & ")"
       Elseif note_notel.Selectionl(0) <> ""Then
5      Print "[/" + note_notel.dbname(O) + "/QuerySelectionOverlayResults?OpenForm&"
       & note_notel.Selection) (0) & "&" & note note2.Moteld & ")"
       Else
       Print "[/" + note_notel.dbname(O) + "lQuerySelectionOverlayResults?OpenForm&"
       & note_note2.Noteld & ")"
10     End If
            End If
       End Sub
```

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SRC Curing Resource dB 4 Query Overlay Open Agent

```
Sub Initialize
        pim ses_ses As New NotesSession
        Dim db db As NotesDatabase
        Dim view-view As NotesView
        Dim note note1 As NotesDocument. note_note2As NotesDocument
        Dim i_cntAs Integer, i addAs Integer

Set db db = ses ses.CurrentDatabase
Set note note1 =ses ses.DocumentContext

S et view-view = db_db. G etView("By N ote1 D ")

If note note1.Selection1(0) <> "" Then
S et note-note2 = view-view. G etD ocumentByKey(R fight("00000000" + note_note1.
S election"! (0). 8))

If Not (note _note2 Is Nothing) Then
        note _note1.data1 = note_note2.EmissData
        note note1.maxfreq1 = note_note2.MaxFreq
End If End If

If note_note1.Selection2(0) <> "" Then
Set note-note2 = view view.GetDocumentByKey(Right("00000000" +
note_note1.Selection2(0), 8))

If Not (note note2 Is Nothing) Then
        note note1.data2=note_note2.EmissData
        note _note1.maxfreq2 = note_note2.MaxFreq
End If End If

If note note1.Selection3(0) <> "" Then
Set note-note2 = view_view.GetDocumentByKey(Right("00000000" +
note_note1.Selection3(0), 8))

If Not (note _note2ls Nothing) Then
        note note1.data3 = note note2.EmissData
        note _note1.maxfreq3=note note2.MaxFreq
        End If End If End Sub
```

```
import java.awt.*; import java.awt.event.*; import java.applet.*;

public class SRC Charts extends Applet { int gi count;

double GetHMax(String str_in) { String str_current; double dbl hmax;

str_current = ""; dblhmax = 0; for Tint i cnt = 0; i_cnt < str_in.length(); i cnt++) {
if(str in. region Match es(i cnt, ", ", 0, 2))
if(Double.valueOf(str current).doubleValue() > dbl_hmax)
dbl hmax = Double.valueOf(str current).doubleValue();
str current = "" ;
i_cnt++;
gi count++; ) else {
str current = str current.concat(str in.substring(i cnt, i cnt + 1));

)
if(str_current.length() > 0) {
        if(Double.valueOf(str_current).doubleValue() > dbl_hmax)
dbl hmax = Double.valueOf(str_current).doubleValue(); gi count++; ) return dbl hmax;


int StringToInt(String str_in, double dbl hmax) { double dbl_pos;

dbl_pos = getSize().height - (25 + (Double.valueOf(str_in).doubleValue() *
((getSize().height - 50) / dbl hmax))); return (int)dbl-pos; )

void drawChartLine(Graphics g, String str_in, String str_type, double dbl_maxfreq) {
double dbl_x, dbl_inc, dbl_hmax; String str last, str next;

str last str_next = "" ; dbl x = 25; gi count = 0;

dbl_hmax = GetHMax(str_in); if(str type. equals IgnoreCase("S")) dbl hmax = 100;

dbl inc = ((((double)getSize().width - 50) / gi count) * ((dbl maxfreq - 200) / 800));
```

```
for (int i cnt = 0; i_cnt < str_in.length(); )   ", ",              i c{
                              nt++)if(str_in.regionMatches(i cnt, 0,
2))if(str_last.length(> 0)      {
                {
g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl inc),
StringToInt(str_next, dbl hmax));
dbl x = dbl x + dbl inc;

str last = str_next; str next = ""; i cnt++;

else { str next = str next.concat(str in.substring(i cnt, i cnt + 1));

)
if(str_next.length() > 0)
g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl-inc),
StringToInt(strnext, dbl_hmax)); )

public void paint(Graphics g) { double dbl x, dbl-y;

g.setColor(Color.black); g.drawLine(0, 0, getSize().width, 0); g.drawLine(25,
getSize().height - 25, getSize().width - 25, getSize().height - 25); g.drawLine(25, 25,
25, getSize().height - 25);

for(int i cnt = 0; i_cnt < 9; i cnt++) {
dbl_x = 25 + ((double)i cnt * (((double)getSize().width - 50) / 8));
g.drawLine((int)dbl x, getSize().height - 25, (int)dbl x, getSize().height - 20);
g.drawString(String.valueOf((i cnt * 100) + 200), (int)dbl x - 8, getSize().height - 5); )

for(int i cnt = 0; i_cnt < 11; i_cnt++) {
dbl-y = 25 + ((double)i cnt * (((double)getSize().height - 50) / 10));
g.drawLine(20, (int)dbl-y, 25, (int)dbl-y);
g.drawString(String.valueOf(100 - (i cnt * 10)), 1, (int)dbl-y + 5); )

g.drawString("Data Overlay", (getSize().width / 2) - 30, 12);

g.setColor(Color.red); drawChartLine(g, getParameter("Data 1 "), getParameter("Type
1 "), Double.valueOf(getParameter("Max Freq 1 ")).doubleValue());
g.setColor(Color.blue); drawChartLine(g, getParameter("Data 2"),
getParameter("Type 2"), Double.valueOf(getParameter("Max Freq
2")).doubleValue()); g.setColor(Color.green); drawChartLine(g, getParameter("Data
3"), getParameter("Type 3"), Double.valueOf(getParameter("Max Freq
3")).doubleValue()); ) )
```
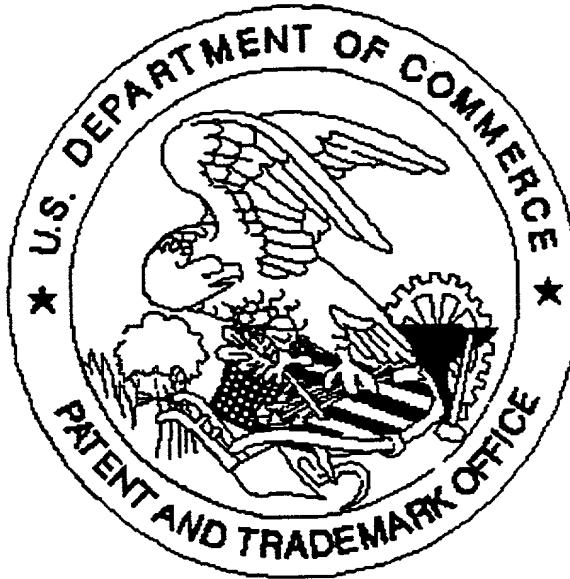
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